Point Interaction Hamiltonians in Bounded Domains

Ph. Blanchard,[*] R. Figari,[†] A. Mantile[‡]

Abstract

Making use of recent techniques in the theory of selfadjoint extensions of symmetric operators, we characterize the class of point interaction Hamiltonians in a 3-D bounded domain with regular boundary. In the particular case of one point interaction acting in the center of a ball, we obtain an explicit representation of the point spectrum of the operator togheter with the corresponding related eigenfunctions. These operators are used to build up a model-system where the dynamics of a quantum particle depends on the state of a quantum bit.

1 Introduction

The name point interactions refers to a particular class of selfadjoint operators obtained as perturbations of the Laplacian supported by discrete sets of points. In $\mathbb{R}^d$, $d \leq 3$, they have been rigorously characterized using the theory of selfadjoint extensions of symmetric operators, [1], and it has been shown, [2], that their spectral properties (eigenvalues and eigenfunctions), and therefore all the physical relevant quantities related to, can be explicitly computed. In this connection, point interactions have been used to build up solvable models for those physical systems where short range forces are supposed to play a role. In spite of their interest in fundamental as well as in applied physics, few results are actually available on this class of interactions in bounded domains (the semigroup generated by a one point interaction in the case of the heat equation in bounded domains is considered in [3]). Making use of recent techniques in the theory of selfadjoint extensions, we give, in the following, a general characterization of point interactions in bounded domains of $\mathbb{R}^3$. In particular we will show that point-supported perturbations of the Laplacian can produce a global change of its spectrum.

The results presented in this work can be used to define model-systems of particles confined in finite regions and interacting with arrays of scattering centers of delta type. Similar models can be used in many different applications and have been already considered in the case of unbounded domains. In particular, our purpose is to provide a model of a finite volume quantum measurement apparatus whose interaction with the system under measurement is described by a delta-shaped quantum potential. An analogous problem in $\mathbb{R}^1$ and $\mathbb{R}^3$ have been investigated in [4].

In the next Section we introduce a classification of the singular perturbations of the Laplacian by means of selfadjoint linear relations (Theorem 4). This parametrization will be used in Section

---

[*]Fakultät für Physik & BiBoS, Universität Bielefeld, D-33501 Bielefeld, Germany. E-mail: blanchard@Physik.Uni-Bielefeld.DE

[†]Istituto Nazionale di Fisica Nucleare (INFN), Sezione di Napoli and Dipartimento Scienze Fisiche, Università degli Studi Napoli "Federico II", Via Cintia, Monte S. Angelo I-80126 Napoli, Italy. E-mail: figari@na.infn.it

[‡]Dipartimento di Matematica e Applicazioni "R. Caccioppoli" Università degli Studi Napoli "Federico II", Via Cintia, Monte S. Angelo I-80126 Napoli, Italy. Supported by a fellowship of Fakültat für Mathematik, Universität Bielefeld, D-33501 Bielefeld, Germany. E-mail: andrea.mantile@dma.unina.it

3 in order to define the selfadjoint operators associated to N point interactions acting in a 3-D bounded domain. In Section 4 one point interaction in a ball is considered: we will show that the symmetry of the system allows, in this case, an explicit computation of the spectral properties of the operator. In Section 5 we define point interactions between a quantum particle and a finite dimensional quantum system. Possible applications of this class of models in the framework of quantum information theory are presented.

2 Parametrization of selfadjoint extensions

We start recalling notation together with few definitions and results in the theory of selfadjoint extensions of symmetric operators in the form introduced in [6].

We consider a closed densely defined symmetric operator, H_0, acting on an Hilbert space $\mathcal{H}$, with deficiency indices (n, n). A triple (V, Γ_1, Γ_2) formed by an auxiliary Hilbert space, V, and a couple of bounded linear operators $\Gamma_{i=1,2} : D(H_0^*) \to V$, such that the following conditions hold[1]:

$$(\psi, H_0^* \varphi) - (H_0^* \psi, \varphi) = \langle \Gamma_1 \psi, \Gamma_2 \varphi \rangle - \langle \Gamma_2 \psi, \Gamma_1 \varphi \rangle \quad \forall \psi, \varphi \in D(H_0^*) \tag{1}$$

$$\text{the map } (\Gamma_1, \Gamma_2) : D(H_0^*) \to V \oplus V \text{ is surjective} \tag{2}$$

defines a *boundary value space* for H_0. This structure, which has been proved to exist for any symmetric operator with equal deficiency indices (see [6], theorem 3.1.5), can be used to parametrize the selfadjoint extensions of H_0 by means of generalized boundary conditions of the form $A\Gamma_1 \psi = B\Gamma_2 \psi$, where A and B are bounded linear operators on V. The conditions to be imposed on the operators A and B, in order that they may describe selfadjoint linear relations, have been given in [5] for any value of the deficiency indices $0 < n \leq \infty$. In particular, for finite values of n, the complex $n \times n$ matrices A, B have to satisfy the properties

$$\begin{array}{ll} [I] & AB^* = BA^* \\ [II] & \text{the } n \times 2n \text{ matrix } (AB) \text{ has maximal rank} \end{array}$$

Denote with W the set of all couples of complex $n \times n$ matrices fulfilling $[I]$ and $[II]$

$$W = \{(A, B) \,|\, [I], [II]\} \tag{3}$$

The following Proposition is an immediate consequence of Theorem 3.1.4 in [6]

Proposition 1 *Let H_0 be a closed symmetric operator with equal deficiency indices (n, n), $n < \infty$, acting on a Hilbert space, and let $(\mathbb{C}^n, \Gamma_1, \Gamma_2)$ be its boundary value space. There is a bijective correspondence between the selfadjoint extensions of H_0 and the set W. A selfadjoint extension $H^{A,B}$, corresponding to $(A, B) \in W$, is given by the restriction of H_0^* to those elements $\psi \in D(H_0^*)$ satisfying the boundary conditions*

$$A\Gamma_1 \psi = B\Gamma_2 \psi \tag{4}$$

In what follows, we will exploit this result to construct selfadjoint operators associated to point perturbations of the Laplacian in bounded domains. We consider the symmetric operator

$$\begin{cases} D(H_0) = \left\{ \psi \in H^2 \cap H_0^1(\Omega) \,\middle|\, \psi|_{\{\underline{x}_k\}_{k=1}^N} = 0 \right\} \\ \\ H_0 \psi = -\Delta \psi \end{cases} \tag{5}$$

---
[1]Here $(\cdot, \cdot)$ and $\langle \cdot, \cdot \rangle$ denotes the scalar products in $L^2(\Omega)$ and V respectively.

where Ω is an open bounded domain of $\mathbb{R}^3$ with regular boundary (for instance $\partial\Omega$ of class C^1 and bounded) and $\{\underline{x}_k\}_{k=1}^N$ is a finite set of points in Ω. The defect spaces of H_0, have the following characterization

Lemma 2 *Let $\mathcal{H}_\pm = Ker\,(\pm i - H_0^*)$ be the defect spaces related to the operator H_0 defined in (5); then*

$$\mathcal{H}_+ = l.s.\left\{\mathcal{G}_0^{-i,k},\ k = 1...N\right\}$$

$$\mathcal{H}_- = l.s.\left\{\mathcal{G}_0^{i,k},\ k = 1...N\right\}$$

where $\mathcal{G}_0^{\pm i,k}$ are the integral kernels of $(-\Delta \pm i)$

$$(-\Delta \pm i)\,\mathcal{G}_0^{\pm i,k} = \delta\,(\cdot - \underline{x}_k) \qquad k = 1...N \tag{6}$$

with Dirichlet conditions on the boundary of Ω, while l.s. denotes the linear span of the sets.

Proof. The spaces $\mathcal{H}_+$ and $\mathcal{H}_-$ are described by the following conditions

$$\psi \in \mathcal{H}_+ \Rightarrow \left\{ \begin{array}{l} (\psi, (\Delta + i)\,\varphi)_{L^2(\Omega)} = 0 \\ \psi \in L^2(\Omega) \end{array} \right. \qquad \forall\varphi \in D(H_0) \tag{7}$$

and

$$\psi \in \mathcal{H}_- \Rightarrow \left\{ \begin{array}{l} (\psi, (\Delta - i)\,\varphi)_{L^2(\Omega)} = 0 \\ \psi \in L^2(\Omega) \end{array} \right. \qquad \forall\varphi \in D(H_0) \tag{8}$$

We analyze the first of these problems. Consider a collection of open balls B_k centered in the points $\{\underline{x}_k\}_{k=1}^N$ with $\cup_{k=1}^N B_k \subset \Omega$ and $B_k \cap B_{k'} = \varnothing \ \forall k \neq k'$. Given any function $\varphi \in H^2 \cap H_0^1(\Omega)$, we define the set U_φ

$$\xi \in U_\varphi \rightarrow \xi(\underline{x}) = \left\{ \begin{array}{ll} 0 & \underline{x} \in \Omega\backslash \cup_{k=1}^N B_k \\ \varphi_k(\underline{x}), & \varphi_k \in \left\{H^2 \cap H_0^1(B_k) \ |\varphi_k(\underline{x}_k) = \varphi(\underline{x}_k)\right\} \end{array} \right. \quad otherwise \tag{9}$$

Given any $\varphi^0 \in D(H_0)$ there are infinitely many $\varphi \in H^2 \cap H_0^1(\Omega)$ coinciding with φ^0 in $\Omega\backslash\cup_{k=1}^N B_k$; for each one of them the difference $\xi_\varphi = \varphi - \varphi^0$ belongs to U_φ. Then the whole domain $D(H_0)$ can be represented in the form

$$\varphi^0 \in D(H_0) \rightarrow \varphi^0 = \varphi - \xi_\varphi \tag{10}$$

by varying φ in $H^2 \cap H_0^1(\Omega)$ and ξ in U_φ. Making use of this representation, equation (7) can be written in the form

$$\left\{ \begin{array}{l} (\psi, (\Delta + i)\,\varphi)_{L^2(\Omega)} - (\psi, (\Delta + i)\,\xi_\varphi)_{L^2(\Omega)} = 0 \\ \psi \in L^2(\Omega) \end{array} \right. \qquad \forall\,(\varphi, \xi) \in H^2 \cap H_0^1(\Omega) \times U_\varphi \tag{11}$$

Due to the essential selfadjointness of the operator $-\Delta$ in the space $H^2 \cap H_0^1(\Omega)$, we know that the equation

$$(\psi, (\Delta + i)\,\varphi)_{L^2(\Omega)} = 0 \qquad \forall\varphi \in H^2 \cap H_0^1(\Omega)$$

has no solution in $L^2(\Omega)$; then there is no ψ for which both terms of (11) are zero. On the other hand, being φ and ξ linked only by their values in the points $\{\underline{x}_k\}_{k=1}^N$, the only non trivial solution of (7) is a linear combination of the Green's functions $\mathcal{G}_0^{-i,k}$ and of their derivatives. Nevertheless we notice that, in the case of 3-D domains, none of the functions $\nabla^n \mathcal{G}_0^{-i,k}$ belongs

3

to $L^2(\Omega)$. The observations above implies that $\mathcal{H}_+$ is an N dimensional space generated by the functions $\left\{\mathcal{G}_0^{-i,k}, \ k = 1...N\right\}$. Proceeding in the same way, it is easy to obtain a similar characterization for $\mathcal{H}_-$, that is: $\mathcal{H}_- = l.s. \left\{\mathcal{G}_0^{i,k}, \ k = 1...N\right\}$. $\blacksquare$

In the following $\mathcal{G}_0^{z,k}$ shall denote the integral kernel of $(-\Delta + z)$ with Dirichlet conditions on the boundary of Ω and centered in the points $\{\underline{x}_k\}_{k=1}^N$; it is worthwhile to recall that these functions are properly defined by[2]

$$\mathcal{G}_0^{z,k}(\underline{x}) = \frac{e^{-\sqrt{z}|\underline{x}-\underline{x}_k|}}{4\pi \, |\underline{x} - \underline{x}_k|} - h_{z,k}(\underline{x}) \tag{12}$$

$$\begin{cases} (-\Delta + z) \, h_{z,k} = 0 \\ h_{z,k}|_{\partial\Omega} = \left. \frac{e^{-\sqrt{z}|\underline{x}-\underline{x}_k|}}{4\pi|\underline{x}-\underline{x}_k|} \right|_{\partial\Omega} \end{cases} \tag{13}$$

whenever $-z$ does not belongs to the point spectrum of the Dirichlet Laplacian in Ω. In Section 3, the asymptotic properties of $h_{z,k}$, as z approaches spectral points, are considered.

Our next task is to defines a couple of operators $\Gamma_{i=1,2} : D(H_0^*) \to \mathbb{C}^N$ such that the triple $\left(\mathbb{C}^N, \Gamma_1, \Gamma_2\right)$ forms a boundary value space for H_0. To this aim, and following the analogous definitions given for the case $\Omega = \mathbb{R}^3$ (see for instance [8]- [10], and [4]), we define

$$(\Gamma_1 \psi)_j = \lim_{\underline{x} \to \underline{x}_j} 4\pi \, |\underline{x} - \underline{x}_j| \, \psi(\underline{x}) \qquad j = 1...N \tag{14}$$

$$(\Gamma_2 \psi)_j = \lim_{\underline{x} \to \underline{x}_j} \left(\psi(\underline{x}) - \frac{(\Gamma_1 \psi)_j}{4\pi \, |\underline{x} - \underline{x}_j|} \right) \qquad j = 1...N \tag{15}$$

Theorem 3 *The triple $\left(\mathbb{C}^N, \Gamma_1, \Gamma_2\right)$ defined by (14) and (15) forms a boundary value space for H_0.*

Proof. The Von Neumann decomposition formula of the domain $D(H_0^*)$ (see for instance [7]) allow us to write the generic vector $\psi \in D(H_0^*)$ in the form

$$\psi = \psi_0 + \sum_{k=1}^N \left(a_k \mathcal{G}_0^{-i,k} + b_k \mathcal{G}_0^{i,k} \right) \qquad a_k, b_k \in \mathbb{C}; \ \psi_0 \in D(H_0) \tag{16}$$

We will use this representation in order to prove that relation (1) holds under our assumptions. Let $\psi, \phi \in D(H_0^*)$ be given by

$$\psi = \psi_0 + \sum_{k=1}^N \left(a_k \mathcal{G}_0^{-i,k} + b_k \mathcal{G}_0^{i,k} \right); \quad \phi = \phi_0 + \sum_{k=1}^N \left(\alpha_k \mathcal{G}_0^{-i,k} + \beta_k \mathcal{G}_0^{i,k} \right) \tag{17}$$

From the symmetry of H_0 it is easy to obtain

$$(\psi, H_0^* \varphi) - (H_0^* \psi, \varphi) = -2i \sum_{k,j=1}^N \left(a_k \alpha_j^* - b_j \beta_k^* \right) \left(\mathcal{G}_0^{-i,k}, \mathcal{G}_0^{-i,j} \right)$$

---

[2]Here and in the following we use $\mathrm{Re} \, \sqrt{z} \geq 0$ as determination of the square root in the complex plane.

Making use of the properties of the functions $\left\{ \mathcal{G}_0^{-i,k} \right\}_{k=1}^N$, we have

$$\left(\mathcal{G}_0^{-i,k}, \mathcal{G}_0^{-i,j} \right) = \begin{cases} -\frac{i}{2} \left(\mathcal{G}_0^{-i,k}(\underline{x}_j) - \mathcal{G}_0^{i,j}(\underline{x}_k) \right) & k \neq j \\ -\operatorname{Re} i h_{i,k}(\underline{x}_k) + \frac{i}{2}\frac{1}{4\pi} \left(\sqrt{-i} - \sqrt{i} \right) & k = j \end{cases}$$

Taking into account that $h_{-i,k} = (h_{i,k})^*$, the previous relation can be written as follows

$$(\psi, H_0^* \varphi) - (H_0^* \psi, \varphi) = -\sum_{k \neq j} \left(a_k \alpha_j^* - b_k \beta_j^* \right) \left(\mathcal{G}_0^{-i,k}(\underline{x}_j) - \mathcal{G}_0^{i,j}(\underline{x}_k) \right) +$$

$$+ \frac{1}{4\pi} \sum_j \left(a_j \alpha_j^* - b_j \beta_j^* \right) \left(\sqrt{-i} - \sqrt{i} \right) + \sum_j \left(a_j \alpha_j^* - b_j \beta_j^* \right) \left(h_{-i,j}(\underline{x}_j) - h_{i,j}(\underline{x}_j) \right) \qquad (18)$$

On the other hand, making use of the representation (16), the action of the operators (14) and (15) is explicitly given by

$$(\Gamma_1 \psi)_j = a_j + b_j \qquad (19)$$

$$(\Gamma_2 \psi)_j = \sum_{\substack{k \\ k \neq j}} a_k \mathcal{G}_0^{-i,k}(\underline{x}_j) + b_k \mathcal{G}_0^{i,k}(\underline{x}_j) - \frac{1}{4\pi} \left[a_j \sqrt{-i} + b_j \sqrt{i} + (\Gamma_1 \psi)_j \right] - a_k h_{-i,j}(\underline{x}_j) - b_k h_{i,j}(\underline{x}_j)$$

$$(20)$$

and the second member of (1) reads as

$$\langle \Gamma_1 \psi, \Gamma_2 \varphi \rangle - \langle \Gamma_2 \psi, \Gamma_1 \varphi \rangle = -\sum_{k \neq j} \left(a_k \alpha_j^* - b_k \beta_j^* \right) \left(\mathcal{G}_0^{-i,k}(\underline{x}_j) - \mathcal{G}_0^{i,j}(\underline{x}_k) \right) +$$

$$- \sum_{k \neq j} a_k \beta_j^* \left(\mathcal{G}_0^{-i,k}(\underline{x}_j) - \mathcal{G}_0^{-i,j}(\underline{x}_k) \right) - \sum_{k \neq j} b_k \alpha_j^* \left(\mathcal{G}_0^{i,k}(\underline{x}_j) - \mathcal{G}_0^{i,j}(\underline{x}_k) \right) +$$

$$+ \frac{1}{4\pi} \sum_j \left(a_j \alpha_j^* - b_j \beta_j^* \right) \left(\sqrt{-i} - \sqrt{i} \right) + \sum_j \left(a_j \alpha_j^* - b_j \beta_j^* \right) \left(h_{-i,j}(\underline{x}_j) - h_{i,j}(\underline{x}_j) \right)$$

Concerning the difference $\mathcal{G}_0^{\pm i,k}(\underline{x}_j) - \mathcal{G}_0^{\pm i,j}(\underline{x}_k)$, from the explicit expression of $\mathcal{G}_0^{\pm i,k}$, follows

$$\mathcal{G}_0^{\pm i,k}(\underline{x}_j) - \mathcal{G}_0^{\pm i,j}(\underline{x}_k) = h_{\pm i,k}(\underline{x}_j) - h_{\pm i,j}(\underline{x}_k)$$

and a simple calculation, exploiting the definition (6), shows that

$$\left(\mathcal{G}_0^{\pm i,k}, \mathcal{G}_0^{\mp i,j} \right) = \left(\mathcal{G}_0^{\pm i,k}, \mathcal{G}_0^{\mp i,j} \right) + i \left(h_{\pm i,k}(\underline{x}_j) - h_{\pm i,j}(\underline{x}_k) \right) \to \left(h_{\pm i,k}(\underline{x}_j) - h_{\pm i,j}(\underline{x}_k) \right) = 0$$

from which we recover

$$(\psi, H_0^* \varphi) - (H_0^* \psi, \varphi) = \langle \Gamma_1 \psi, \Gamma_2 \varphi \rangle - \langle \Gamma_2 \psi, \Gamma_1 \varphi \rangle$$

The proof of (2) easily follows from definitions (19) and (20). ∎

The above result allows a general characterization of the selfadjoint extensions of operator H_0 in terms of selfadjoint boundary conditions. From Proposition 1, any selfadjoint extension of H_0 can be parametrized through an element of the set W (see definition (3)); the one corresponding to the couple $(A, B) \in W$ is given by the restriction of H_0^* to those elements $\psi \in D(H_0^*)$ which satisfy the boundary conditions (4). Denoting with H^{AB} this extension, we have

$$D(H^{AB}) = \{ \psi \in D(H_0^*) \,|\, A\Gamma_1 \psi = B\Gamma_2 \psi \} \qquad (21)$$

$$H^{AB}\psi = H_0^*\psi \tag{22}$$

The next theorem gives an explicit representation of the domain and provide a resolvent formula for any operator of type (21)-(22).

Theorem 4 *Fix $(A, B) \in W$, let H^{AB} - defined by (21)-(22) - be the related extension and R_z^{AB} its resolvent. For any $\lambda \in \mathbb{C}\backslash\mathbb{R}$, the following representation holds*

$$D(H^{AB}) = \left\{ \psi \in L^2(\Omega) \middle| \ \psi = \phi^\lambda + \sum_{k=1}^N q_k \mathcal{G}_0^{\lambda,k}, \ \phi^\lambda \in H^2 \cap H_0^1(\Omega), \right.$$
$$\left. q_j = (\Gamma_1\psi)_j , \ \sum_j B_{kj}\phi^\lambda(\underline{x}_j) = \sum_j (B\,\Gamma(\lambda) + A)_{kj}\,q_j \right\} \tag{23}$$

$$H^{AB}\psi = -\Delta\phi - \lambda\sum_{k=1}^N q_k \mathcal{G}_0^{\lambda,k} \tag{24}$$

$$R_z^{AB}\varphi = R_z\varphi + \sum_{j,l,k=1}^N (B\Gamma(z) + A)_{jl}^{-1}\, B_{lk}\, R_z\varphi(\underline{x}_k)\, \mathcal{G}_0^{z,j}, \quad \forall\varphi \in L^2(\Omega), \ z \in \mathbb{C}\backslash\mathbb{R} \tag{25}$$

$$\Gamma_{kj}(z) = \begin{cases} -\mathcal{G}_0^{z,j}(\underline{x}_k) & j \neq k \\ h_{z,k}(\underline{x}_k) + \frac{\sqrt{z}}{4\pi} & j = k \end{cases} \tag{26}$$

where $R_z = \frac{1}{-\Delta+z}$ is the resolvent operator associated to $-\Delta$ with Dirichlet boundary conditions in Ω.

Proof. As follows from the decomposition formula (16), the generic vector in the domain $D(H_0^*)$ has the form $\psi = \psi_0 + \sum_{k=1}^N \left(a_k \mathcal{G}_0^{-i,k} + b_k \mathcal{G}_0^{i,k} \right)$ with $\psi_0 \in D(H_0)$. Fix $\lambda \in \mathbb{C}\backslash\mathbb{R}$ and set ϕ^λ

$$\phi^\lambda = \psi_0 + \sum_{k=1}^N \left(a_k \mathcal{G}_0^{-i,k} + b_k \mathcal{G}_0^{i,k} \right) - \sum_{k=1}^N q_k \mathcal{G}_0^{\lambda,k} \tag{27}$$

$$q_j = (\Gamma_1\psi)_j = a_j + b_j \tag{28}$$

Our first task is to show that $\phi^\lambda \in H^2 \cap H_0^1(\Omega)$; to this aim we notice that $\phi^\lambda \in H^2 \cap H_0^1(\Omega\backslash\{\underline{x}_k\}_{k=1}^N)$, so that the set of its singular points is contained in $\{\underline{x}_k\}_{k=1}^N$. Taking into account the explicit expressions of the Green functions $\mathcal{G}_0^{z,k}$, it is easy to see that, apart from regular terms, ϕ^λ behaves around $\underline{x}_{\bar{k}} \in \{\underline{x}_k\}_{k=1}^N$ as

$$\phi_{s,\bar{k}}(\underline{x}) = a_{\bar{k}}\frac{e^{-\sqrt{-i}|\underline{x}-\underline{x}_{\bar{k}}|}}{4\pi\,|\underline{x}-\underline{x}_{\bar{k}}|} + b_{\bar{k}}\frac{e^{-\sqrt{i}|\underline{x}-\underline{x}_{\bar{k}}|}}{4\pi\,|\underline{x}-\underline{x}_{\bar{k}}|} - q_{\bar{k}}\frac{e^{-\sqrt{\lambda}|\underline{x}-\underline{x}_{\bar{k}}|}}{4\pi\,|\underline{x}-\underline{x}_{\bar{k}}|}$$

A direct calculation shows that $\phi_{s,\bar{k}}$ and $\nabla\phi_{s,\bar{k}}$ both have finite values in the limit $\underline{x} \to \underline{x}_{\bar{k}}$

$$\lim_{\underline{x}\to\underline{x}_{\bar{k}}} \phi_{s,\bar{k}} = -\frac{1}{4\pi}\left[a_{\bar{k}}\sqrt{-i} + b_{\bar{k}}\sqrt{i} - q_{\bar{k}}\sqrt{\lambda} \right] \tag{29}$$

$$\lim_{\underline{x}\to\underline{x}_{\bar{k}}} \nabla\phi_{s,\bar{k}} = \hat{r}_{\bar{k}}\frac{1}{8\pi}\left[a_{\bar{k}}\sqrt{-i} + b_{\bar{k}}\sqrt{i} - q_{\bar{k}}\lambda \right] \tag{30}$$

with $\hat{r}_{\bar{k}} = \frac{\underline{x}_{\bar{k}}}{|\underline{x}_{\bar{k}}|}$. Moreover, a compensation mechanism avoid the function $\Delta\phi_{s,\bar{k}}$ to have purely distributional terms. Infact, making use of the equation

$$(-\Delta + z)\frac{e^{-\sqrt{z}|\underline{x}-\underline{x}_k|}}{4\pi\,|\underline{x}-\underline{x}_k|} = \delta\left(\underline{x} - \underline{x}_k\right)$$

6

holding for all $z \in \mathbb{C} \backslash \{\lambda_n\}_{n \in \mathbb{N}}$, we have

$$
\Delta \phi_{s,\bar{k}} = \Delta \left[a_{\bar{k}} \frac{e^{-\sqrt{-i}|\underline{x}-\underline{x}_{\bar{k}}|}}{4\pi |\underline{x} - \underline{x}_{\bar{k}}|} + b_{\bar{k}} \frac{e^{-\sqrt{i}|\underline{x}-\underline{x}_{\bar{k}}|}}{4\pi |\underline{x} - \underline{x}_{\bar{k}}|} - q_{\bar{k}} \frac{e^{-\sqrt{\lambda}|\underline{x}-\underline{x}_{\bar{k}}|}}{4\pi |\underline{x} - \underline{x}_{\bar{k}}|} \right] =
$$

$$
= -a_{\bar{k}} i \frac{e^{-\sqrt{-i}|\underline{x}-\underline{x}_{\bar{k}}|}}{4\pi |\underline{x} - \underline{x}_{\bar{k}}|} + b_{\bar{k}} i \frac{e^{-\sqrt{i}|\underline{x}-\underline{x}_{\bar{k}}|}}{4\pi |\underline{x} - \underline{x}_{\bar{k}}|} - q_{\bar{k}} \lambda \frac{e^{-\sqrt{\lambda}|\underline{x}-\underline{x}_{\bar{k}}|}}{4\pi |\underline{x} - \underline{x}_{\bar{k}}|} + (-a_{\bar{k}} - b_{\bar{k}} + q_{\bar{k}}) \delta(\underline{x} - \underline{x}_k)
$$

From (28) it follows that $\Delta \phi_{s,\bar{k}} \in L^2(\Omega)$. The previous observations imply that $\phi^\lambda \in H^2 \cap H_0^1(S)$; this result guarantees the equivalence of the representations

$$
\psi = \psi_0 + \sum_{k=1}^{N} \left(a_k \mathcal{G}_0^{-i,k} + b_k \mathcal{G}_0^{i,k} \right), \quad \psi_0 \in D(H_0) \tag{31}
$$

and

$$
\psi = \phi^\lambda + \sum_{k=1}^{N} q_k \mathcal{G}_0^{\lambda,k}, \quad \lambda \in \mathbb{C} \backslash \mathbb{R}^+, \ \phi^\lambda \in H^2 \cap H_0^1(S) \tag{32}
$$

of the domain $D(H_0^*)$.

From (29) and making use of the explicit expression (12)-(27), it follows that any ψ in (23) obeys to the relation $\phi^\lambda(\underline{x}_k) = \Gamma_{kj}(\lambda)q_j + (\Gamma_2 \psi)_k$, with $\Gamma_{kj}(\lambda)$ given by (26) and $q_j = (\Gamma_1 \psi)_j$; taking into account the boundary relations $A\Gamma_1\psi = B\Gamma_2\psi$, we get the following characterization of the values of ϕ^λ in the points $\underline{x}_k$

$$
\sum_j B_{kj} \phi^\lambda(\underline{x}_j) = \sum_j (B\,\Gamma(\lambda) + A)_{kj} \, q_j \tag{33}
$$

Relations (32)-(33) identify the alternative representation of the domain $D(H^{AB})$ given in (23).

Let $\psi = \phi^\lambda + \sum_{k=1}^{N} q_k \mathcal{G}_0^{\lambda,k}$: from the definition (22), we get for the action of operator H^{AB}

$$
\left(H^{AB}\psi, \varphi \right) = \left(\phi^\lambda, H_0\varphi \right) + \left(\sum_{k=1}^{N} q_k \mathcal{G}_0^{\lambda,k}, H_0\varphi \right)
$$

then an integration by parts easily shows that $H^{AB}\psi$ is described by the relation (24).

The resolvent R_z^{AB} associated to the operator H^{AB}, for $z \in \mathbb{C} \backslash \mathbb{R}$, is a bounded linear map: $L^2(\Omega) \to D(H^{AB})$. Let $\varphi \in L^2(\Omega)$, exploiting the regularity of the map $R_z \in \mathcal{B}(L^2(\Omega), H^2 \cap H_0^1(\Omega))$, we can identify with $R_z\varphi$ the H^2-part of the function $R_z^{AB}\varphi$; therefore, from (32)-(33), the function $R_z^{AB}\varphi \in D(H^{AB})$ has the following representation

$$
R_z^{AB}\varphi = R_z\varphi + \sum_{k=1}^{N} q_k(\varphi) \mathcal{G}_0^{z,k}
$$

$$
\sum_j B_{kj} R_z\varphi(\underline{x}_j) = \sum_{l,j} B_{kl}\Gamma_{lj}(z)q_j(\varphi) + \sum_j A_{kj}q_j(\varphi)
$$

from which it follows

$$
q_j(\varphi) = \sum_{l,k} (B\Gamma(z) + A)_{jl}^{-1} B_{lk} R_z\varphi(\underline{x}_k) \tag{34}
$$

∎

3   Point interactions operators in bounded domains

The family of extensions described by (23)-(24) include both the, so called, local and non local point interactions. The interaction type is specified by the boundary conditions (4); from the definitions of Γ_1 and Γ_2 it follows that the asymptotics of $\psi \in D\left(H_0^*\right)$ as $\underline{x} \to \underline{x}_k$ is given by

$$\psi \underset{\underline{x} \to \underline{x}_k}{\sim} \frac{1}{4\pi \left|\underline{x} - \underline{x}_k\right|} (\Gamma_1 \psi)_k + (\Gamma_2 \psi)_k + o(1)$$

then, through the relation $A\Gamma_1 \psi = B\Gamma_2 \psi$, a link between the asymptotic behavior of the singular and the regular part of the state ψ is established. Whenever the coefficient of the singularity in the point $\underline{x}_k$, $(\Gamma_1 \psi)_k$, depends only on the value in $\underline{x}_k$ of the regular part of ψ, i.e on $(\Gamma_2 \psi)_k$, the interaction will be said to be local. This condition is obtained by requiring the matrices A and B to be diagonal. Without loss of generality, we can parametrize the most general extension of local kind using a set of N real, $\{\alpha_k\}_{k=1}^N$, such that

$$A_{ij} = \alpha_i\, \delta_{ij}, \quad B_{ij} = \delta_{ij} \tag{35}$$

Under this assumption, we shall investigate some spectral properties of operators H^{AB}. Taking in account (35), the resolvent formula (25) can be written as

$$R_z^{AB} \varphi = R_z \varphi + \sum_{j,k=1}^N (\Gamma(z) + A)_{jk}^{-1}\, R_z \varphi(\underline{x}_k)\, \mathcal{G}_0^{z,j} \tag{36}$$

with

$$(\Gamma(z) + A)_{kj} = \begin{cases} -\mathcal{G}_0^{z,j}(\underline{x}_k) & j \neq k \\ \alpha_k + h_{z,k}(\underline{x}_k) + \frac{\sqrt{z}}{4\pi} & j = k \end{cases} \tag{37}$$

In what follows, we shall make use of the spectral properties of the Laplacian operator defined in $H^2 \cap H_0^1(\Omega)$. Let us denote with $\{\lambda_n\}_{n\in\mathbb{N}}$ the spectral points of $-\Delta$ with Dirichlet boundary conditions in Ω. We shall assume each eigenvalue λ_n to have a degeneracy M_n; the normalized eigenvectors related to λ_n, denoted with $\{\phi_{n,m}\}_{m=1}^{M_n}$, satisfy the equations

$$\begin{cases} (H - \lambda_n)\, \phi_{n,m} = 0 \\ \phi_{n,m}|_{\partial\Omega} = 0; \qquad \|\phi_{n,m}\|_{L^2(\Omega)} = 1 \end{cases} \tag{38}$$

These vectors span an M_n dimensional space in $H^2 \cap H_0^1(\Omega)$.

The resolvent operator $R_z = \frac{1}{-\Delta + z}$ is a bounded map: $L^2(\Omega) \to H^2 \cap H_0^1(\Omega)$ whose action on a vector φ can be represented as follows

$$R_z \varphi = \sum_{n\in\mathbb{N}} \sum_{m=1}^{M_n} \frac{(\varphi, \phi_{n,m})}{\lambda_n + z} \phi_{n,m} \tag{39}$$

The next Lemma gives a general characterization of the asymptotic behavior of the functions $h_{z,k}$ as z approximates a point in the spectrum of operator $-\Delta$.

Lemma 5 *Let $\lambda_{\bar{n}}$ be an eigenvalue of the operator $-\Delta$ - defined on $H^2 \cap H_0^1(\Omega)$ - and $\phi_{\bar{n},m}$ be the corresponding eigenfunctions and $h_{z,k}$ defined by (13); then the following limit holds*

$$\lim_{|\varepsilon|\to 0} \left\| \varepsilon h_{-\lambda_{\bar{n}}+\varepsilon,\, k} + \sum_{m=1}^{M_{\bar{n}}} \phi_{\bar{n},m}^*(\underline{x}_k)\, \phi_{\bar{n},m} \right\|_{L^2(\Omega)} = 0 \tag{40}$$

with $\varepsilon \in \mathbb{C}$.

Proof. From definition (12), we get

$$\left\| \varepsilon h_{-\lambda_{\bar{n}}+\varepsilon,\,k} + \sum_{m=1}^{M_{\bar{n}}} \phi_{\bar{n},m}^*(\underline{x}_k)\,\phi_{\bar{n},m} \right\|_{L^2(\Omega)} \leq |\varepsilon| \left\| \frac{e^{-\sqrt{z}|\underline{x}-\underline{x}_k|}}{4\pi\,|\underline{x}-\underline{x}_k|} \right\|_{L^2(\Omega)} + |\varepsilon| \left\| \mathcal{G}_0^{-\lambda_{\bar{n}}+\varepsilon,\,k} - \sum_{m=1}^{M_{\bar{n}}} \frac{\phi_{\bar{n},m}^*(\underline{x}_k)\,\phi_{\bar{n},m}}{\varepsilon} \right\|_{L^2(\Omega)}$$

The first contribution at the r.h.s. of this expression is clearly an $O(\varepsilon)$ being $\frac{e^{-\sqrt{z}|\underline{x}-\underline{x}_k|}}{4\pi|\underline{x}-\underline{x}_k|} \in L^2(\Omega)$.

Concerning the second contribution, we notice that $\mathcal{G}_0^{z,k} - \sum_{m=1}^{M_n} \frac{\phi_{\bar{n},m}^*(\underline{x}_k)\,\phi_{\bar{n},m}}{\lambda_{\bar{n}}+z}$ is the value in $\underline{x}_k$ of the integral kernel of the operator $(-\Delta + z)^{-1}$ restricted to the space $L^2(\Omega)\backslash l.s\,\{\phi_{\bar{n},m}\}_{m=1}^{M_{\bar{n}}}$. It belongs to $L^2(\Omega)\backslash l.s\,\{\phi_{\bar{n},m}\}_{m=1}^{M_{\bar{n}}}$ for all $\underline{x}_k \in \Omega$ and $z \in \mathbb{C}\backslash\{-\lambda_n\}_{\substack{n\in\mathbb{N}\\ n\neq\bar{n}}}$, it follows that

$$\lim_{z\to\lambda_{\bar{n}}} \left\| \mathcal{G}_0^{z,k} - \sum_{m=1}^{M_n} \frac{\phi_{\bar{n},m}^*(\underline{x}_k)\,\phi_{\bar{n},m}}{\lambda_{\bar{n}}+z} \right\|_{L^2(\Omega)} < \infty$$

which implies

$$\lim_{|\varepsilon|\to 0} |\varepsilon| \left\| \mathcal{G}_0^{-\lambda_{\bar{n}}+\varepsilon,\,k} - \sum_{m=1}^{M_{\bar{n}}} \frac{\phi_{\bar{n},m}^*(\underline{x}_k)\,\phi_{\bar{n},m}}{\varepsilon} \right\|_{L^2(\Omega)} = 0$$

∎

Making use of the previous Lemma, we study the behavior of $R_z^{AB}\varphi$, $\varphi \in L^2(\Omega)$, as z approaches non-degenerate spectral points of $-\Delta$.

Theorem 6 *Let $\lambda_{\bar{n}}$ be a non-degenerate eigenvalue of the operator $-\Delta$ defined on $H^2 \cap H_0^1(\Omega)$, and assume the corresponding eigenfunction $\phi_{\bar{n}}$ satisfies the following condition*

$$\phi_{\bar{n}}(\underline{x}_k) \neq \underline{0} \in \mathbb{C}^N$$

then for any $\varphi \in L^2(\Omega)$, the limit $\lim_{z\to-\lambda_{\bar{n}}} R_z^{AB}\varphi$ belongs to $L^2(\Omega)$.

Proof. Our aim is to prove that the point $-\lambda_{\bar{n}}$ is not a singular point for R_z^{AB}. From the explicit expression of $R_z\varphi$ (see the representation (39) above), it follows that

$$R_z^{AB}\varphi = \sum_{n\in\mathbb{N}} \sum_{m=1}^{M_n} \frac{(\varphi,\phi_{n,m})}{\lambda_n+z} \phi_{n,m} + \sum_{n\in\mathbb{N}} \sum_{m=1}^{M_n} \frac{(\varphi,\phi_{n,m})}{\lambda_n+z} \sum_{j,k=1}^{N} (\Gamma(z)+A)_{jk}^{-1}\,\phi_{n,m}(\underline{x}_k)\,\mathcal{G}_0^{z,j} \quad (41)$$

Set $z = -\lambda_{\bar{n}} + \varepsilon$, $\varepsilon \in \mathbb{C}$; we shall denote with $\left[R_{-\lambda_{\bar{n}}+\varepsilon}^{AB}\varphi\right]_s$ the singular part of $R_{-\lambda_{\bar{n}}+\varepsilon}^{AB}\varphi$ for $|\varepsilon| \to 0$; this function is given by

$$\left[R_{-\lambda_{\bar{n}}+\varepsilon}^{AB}\varphi\right]_s = \frac{(\varphi,\phi_{\bar{n}})}{\varepsilon} \phi_{\bar{n}} + \frac{(\varphi,\phi_{\bar{n}})}{\varepsilon} \sum_{j,k=1}^{N} (\Gamma(-\lambda_{\bar{n}}+\varepsilon)+A)_{jk}^{-1}\,\phi_{\bar{n}}(\underline{x}_k)\,\mathcal{G}_0^{-\lambda_{\bar{n}}+\varepsilon,\,j} \quad (42)$$

Replacing $\mathcal{G}_0^{-\lambda_{\bar{n}}+\varepsilon,\,j}$ with (12), from the previous expression we get

$$\left[R_{-\lambda_{\bar{n}}+\varepsilon}^{AB}\varphi\right]_s = (\varphi,\phi_{\bar{n}}) \sum_{j,k=1}^{N} \frac{(\Gamma(-\lambda_{\bar{n}}+\varepsilon)+A)_{jk}^{-1}}{\varepsilon} \phi_{\bar{n}}(\underline{x}_k) \frac{e^{-\sqrt{-\lambda_{\bar{n}}+\varepsilon}|\cdot-\underline{x}_j|}}{4\pi\,|\cdot-\underline{x}_j|} +$$

$$+ \frac{(\varphi,\phi_{\bar{n}})}{\varepsilon} \left[\phi_{\bar{n}} - \sum_{j,k=1}^{N} (\Gamma(-\lambda_{\bar{n}}+\varepsilon)+A)_{jk}^{-1}\,\phi_{\bar{n}}(\underline{x}_k)\,h_{-\lambda_{\bar{n}}+\varepsilon,\,j} \right] \quad (43)$$

We will study the two contributions in (43) separately.

9

1. Define the vector $u_j^\varepsilon \in \mathbb{C}^N$ in the following way

$$\phi_{\bar{n}}(\underline{x}_k) = \sum_j \varepsilon \left(\Gamma(-\lambda_{\bar{n}} + \varepsilon) + A\right)_{kj} u_j^\varepsilon \tag{44}$$

Using the relation (40) with $M_{\bar{n}} = 1$, we have

$$\lim_{|\varepsilon| \to 0} \varepsilon \left(\Gamma(-\lambda_{\bar{n}} + \varepsilon) + A\right)_{kj} = \begin{cases} -\phi_{\bar{n}}^*(\underline{x}_j)\phi_{\bar{n}}(\underline{x}_k) & j \neq k \\ -|\phi_{\bar{n}}(\underline{x}_k)|^2 & j = k \end{cases} \tag{45}$$

then, limit of (44) as $|\varepsilon| \to 0$ is given by

$$\phi_{\bar{n}}(\underline{x}_k) = -\phi_{\bar{n}}(\underline{x}_k) \sum_j \phi_{\bar{n},}^*(\underline{x}_j) u_j^0 \tag{46}$$

from which it follows

$$-\sum_j \phi_{\bar{n},m'}^*(\underline{x}_j) u_{j,m}(0) = 1 \tag{47}$$

Under the assumption $\phi_{\bar{n}}(\underline{x}_k) \neq \underline{0}$, condition (47) defines a subset of vectors $u_j^0 \in \mathbb{C}^N$ whose scalar product with $\phi_{\bar{n}}(\underline{x}_j)$ is equal to 1. We conclude that, in the limit $|\varepsilon| \to 0$, the first contribution at the r.h.s. of (43) is given by $(\varphi, \phi_{\bar{n}}) \sum_{j=1}^N u_j^0 \frac{e^{-\sqrt{-\lambda_{\bar{n}} + \varepsilon}|\cdot - x_j|}}{4\pi|\cdot - \underline{x}_j|}$ which is clearly in $L^2(\Omega)$.

2. We use definition (44), in order to write the second term at the r.h.s. of (43) as

$$\frac{(\varphi, \phi_{\bar{n}})}{\varepsilon} \left[\phi_{\bar{n}} - \sum_{j=1}^N u_j^\varepsilon \varepsilon h_{-\lambda_{\bar{n}} + \varepsilon, j}\right] \tag{48}$$

From (40) and the previous result (47), it follows

$$\lim_{|\varepsilon| \to 0} \left[\phi_{\bar{n}} - \sum_{j=1}^N u_j^\varepsilon \varepsilon h_{-\lambda_{\bar{n}} + \varepsilon, j}\right] = 0 \tag{49}$$

In order to study the behavior of (48) as $|\varepsilon| \to 0$, we need to define the derivative $\frac{d}{d\varepsilon} u_j^\varepsilon$ for $\varepsilon = 0$; to this aim we notice that from relation (44) it follows

$$\sum_j \varepsilon \left(\Gamma(-\lambda_{\bar{n}} + \varepsilon) + A\right)_{kj} \frac{d}{d\varepsilon} u_j^\varepsilon = -\sum_j \frac{d}{d\varepsilon} \left[\varepsilon \left(\Gamma(-\lambda_{\bar{n}} + \varepsilon) + A\right)_{kj}\right] u_j^\varepsilon \tag{50}$$

Being

$$\frac{d}{d\varepsilon} \left[\varepsilon \left(\Gamma(-\lambda_{\bar{n}} + \varepsilon) + A\right)_{kj}\right]\bigg|_{\varepsilon=0} = \begin{cases} \lim_{|\varepsilon| \to 0} \frac{d}{d\varepsilon} \varepsilon h_{z,j}(\underline{x}_k) & j \neq k \\ \alpha_k + \lim_{|\varepsilon| \to 0} \frac{d}{d\varepsilon} \varepsilon h_{z,k}(\underline{x}_k) & j = k \end{cases} \tag{51}$$

and using (45), we obtain

$$-\sum_j \phi_{\bar{n}}^*(\underline{x}_j)\phi_{\bar{n}}(\underline{x}_k) \frac{d}{d\varepsilon} u_j^\varepsilon\bigg|_{\varepsilon=0} = -\sum_j \left(\lim_{|\varepsilon| \to 0} \frac{d}{d\varepsilon} \varepsilon h_{z,j}(\underline{x}_k) + \alpha_k \delta_{jk}\right) u_j^0 \tag{52}$$

10

Due to the arbitrariness in the choice of $\underline{x}_k$, we may intend the previous relation in a local sense

$$-\sum_j \phi_{\bar{n}}^*(\underline{x}_j)\phi_{\bar{n}}(\underline{x}) \left.\frac{d}{d\varepsilon}u_j^\varepsilon(\underline{x})\right|_{\varepsilon=0} = -\sum_j \left(\lim_{|\varepsilon|\to 0}\frac{d}{d\varepsilon}\varepsilon h_{z,j}(\underline{x}) + \alpha_k\delta_{jk}\right)u_j^0(\underline{x}) \qquad (53)$$

where $\underline{x} \in \{\underline{x}_k\}_{k=1}^N$ and $u_j^\varepsilon(\underline{x}) \in L^2(\Omega)$ is defined by (44). Next we evaluate the limit $|\varepsilon| \to 0$ of the function (48)

$$\lim_{|\varepsilon|\to 0}\frac{(\varphi,\phi_{\bar{n}})}{\varepsilon}\left[\phi_{\bar{n}} - \sum_{j=1}^N u_j^\varepsilon\,\varepsilon h_{-\lambda_{\bar{n}}+\varepsilon,\,j}\right] = -(\varphi,\phi_{\bar{n}})\lim_{|\varepsilon|\to 0}\frac{d}{d\varepsilon}\sum_{j=1}^N u_j^\varepsilon\,\varepsilon h_{-\lambda_{\bar{n}}+\varepsilon,\,j} =$$

$$= (\varphi,\phi_{\bar{n}})\left(\sum_{j=1}^N \phi_{\bar{n}}^*(\underline{x}_j)\phi_{\bar{n}}\lim_{|\varepsilon|\to 0}\frac{d}{d\varepsilon}u_j^\varepsilon - \sum_{j=1}^N u_j^\varepsilon\lim_{|\varepsilon|\to 0}\frac{d}{d\varepsilon}\varepsilon h_{-\lambda_{\bar{n}}+\varepsilon,\,j}\right)$$

Exploiting (53), we obtain an $L^2(\Omega)$ function

$$\lim_{|\varepsilon|\to 0}\frac{(\varphi,\phi_{\bar{n}})}{\varepsilon}\left[\phi_{\bar{n}} - \sum_{j=1}^N u_j^\varepsilon\,\varepsilon h_{-\lambda_{\bar{n}}+\varepsilon,\,j}\right] = (\varphi,\phi_{\bar{n}})\sum_j \alpha_j\,u_j^0 \qquad (54)$$

∎

4 One point interaction in the ball: an exact solvable model

In this section we shall study the selfadjoint extensions of H_0 when Ω is a ball of radius R, centered in the origin of $\mathbb{R}^3$. With the notation of the previous section, we will consider the case

$$N = 1,\ \underline{x}_1 = \underline{0},\ A = \alpha \in \mathbb{R},\ B = 1 \qquad (55)$$

With this choice of parameters, the operator H^{AB} describes a point interaction acting in the origin of Ω; in what follows it will be denoted as H_α.

In order to characterize the spectral properties of H_α, we preliminary recall some basic facts about the Laplacian operator in the ball. Set $\mathbb{N}_0 \equiv \mathbb{N} \cup \{0\}$ and let $\{\lambda_{n,k}\}_{n\in\mathbb{N}_0,\,k\in\mathbb{N}}$ be the point spectrum of $-\Delta$ in the ball Ω with homogeneous Dirichlet conditions boundary: it is well known that, for fixed n, the $\lambda_{n,k}$ are positive and $2n+1$ times degenerate; the corresponding eigenfuctions $\{\psi_{n,m,k},\ n\in\mathbb{N}_0,\ m\in\mathbb{Z}\cap[-n,n],\ k\in\mathbb{N}\}$ form a basis for the space $L^2(\Omega)$. A general expression of $\psi_{n,m,k}$ in polar coordinates is

$$\psi_{n,m,k}(r,\vartheta,\varphi) = j_n(\sqrt{\lambda_{n,k}}\,r)\,Y_{n,m}(\vartheta,\varphi) \qquad (56)$$

where the radial part is given in terms of the spherical Bessel functions of order n, j_n, and the angular part is a combination of spherical harmonics. For any $n \in \mathbb{N}_0$, the values $\lambda_{n,k}$ are fixed by the boundary condition

$$j_n(\sqrt{\lambda_{n,k}}\,R) = 0 \qquad (57)$$

From relations (23)-(26) in Theorem 4 and form assumptions (55) we get the following representation

$$D(H_\alpha) = \left\{\psi \in L^2(\Omega)\,\big|\,\psi = \phi^\lambda + q\mathcal{G}_0^\lambda\,,\ \phi^\lambda \in H^2 \cap H_0^1(\Omega),\right.$$

$$\left.\phi^\lambda(\underline{0}) = q\left(\alpha + \frac{\sqrt{\lambda}}{4\pi} + h_\lambda(\underline{0})\right),\ \lambda \in \mathbb{C}\backslash\{\lambda_{n,k}\}_{n\in\mathbb{N}_0,\,k\in\mathbb{N}}\right\} \qquad (58)$$

$$H_\alpha \psi = -\Delta \phi^\lambda - \lambda q \mathcal{G}_0^\lambda \tag{59}$$

$$R_z^\alpha \varphi = R_z \varphi + \frac{R_z \varphi(\underline{0})}{\alpha + \frac{\sqrt{z}}{4\pi} + h_z(\underline{0})} \mathcal{G}_0^z \tag{60}$$

with

$$\mathcal{G}_0^z(\underline{x}) = \frac{e^{-\sqrt{z}|\underline{x}|}}{4\pi |\underline{x}|} - h_z(\underline{x}) \tag{61}$$

$$\begin{cases} (-\Delta + z) \, h_z = 0 \\ h_z|_{\partial\Omega} = \frac{e^{-\sqrt{z}R}}{4\pi R} \end{cases} \tag{62}$$

As it was stressed in the previous section, the action of operator R_z can be expressed by means of the eigenfuctions of the Dirichlet Laplacian in Ω

$$R_z \varphi = \sum_{\substack{n \in \mathbb{N}_0 \\ m \in \mathbb{Z} \cap [-n,n] \\ k \in \mathbb{N}}} \frac{(\varphi, \psi_{n,m,k})}{\lambda_{n,k} + z} \psi_{n,m,k} \tag{63}$$

Replacing (63) into (60) we get

$$R_z^\alpha \varphi = \sum_{\substack{n \in \mathbb{N}_0 \\ m \in \mathbb{Z} \cap [-n,n] \\ k \in \mathbb{N}}} \frac{(\varphi, \psi_{n,m,k})}{\lambda_{n,k} + z} \psi_{n,m,k} + \sum_{\substack{n \in \mathbb{N}_0 \\ m \in \mathbb{Z} \cap [-n,n] \\ k \in \mathbb{N}}} \frac{(\varphi, \psi_{n,m,k})}{\lambda_{n,k} + z} \frac{\psi_{n,m,k}(\underline{0})}{\alpha + \frac{\sqrt{z}}{4\pi} + h_z(\underline{0})} \mathcal{G}_0^z \tag{64}$$

The explicit knowledge of the system $\{\psi_{n,m,k}\}$, will allow a direct calculation of the spectral properties of H_α. The Fourier expansion of $\mathcal{G}_0^z$ in terms of the vectors $\psi_{n,k}$ is: $\mathcal{G}_0^z = \sum_{n,m,k} \frac{\psi_{n,m,k}^*(\underline{0})}{\lambda_{n,k} + z} \psi_{n,m,k}$; the relation

$$j_n(0) = \begin{cases} 0 & n \neq 0 \\ 1 & n = 0 \end{cases} \tag{65}$$

implies: $\psi_{n,m,k}^*(\underline{0}) = \delta_{n\,0}$, and a simplified expression of $\mathcal{G}_0^z$ follows

$$\mathcal{G}_0^z = \sum_{k \in \mathbb{N}} \frac{\psi_{0,0,k}}{\lambda_{0,k} + z} \tag{66}$$

From (66) one can deduce an explicit form of the solution of (62). Infact, using the definition (61), we have

$$h_z(r, \vartheta, \varphi) = \frac{e^{-\sqrt{z}r}}{4\pi r} - \sum_{k \in \mathbb{N}} \frac{\psi_{0,0,k}(r)}{\lambda_{0,k} + z} \tag{67}$$

Moreover, as a direct calculation shows, for any $z \in \mathbb{C} \setminus \{-\lambda_{n,k}\}_{n \in \mathbb{N}_0, \, k \in \mathbb{N}}$ the expansion of the function $\frac{e^{-\sqrt{z}r}}{4\pi r}$ w.r.t. the system $\{\psi_{n,m,k}\}$ is

$$\frac{e^{-\sqrt{z}r}}{4\pi r} = \sum_{k \in \mathbb{N}} \frac{\psi_{0,0,k}^*(\underline{0})}{\lambda_{0,k} + z} \psi_{0,0,k}(r) - \frac{e^{-\sqrt{z}R}}{4\pi R} \frac{j_0(\sqrt{-z}\,r)}{j_0(\sqrt{-z}\,R)} \tag{68}$$

Replacing this expression in (67), we get

$$\forall z \in \mathbb{C} \setminus \{-\lambda_{n,k}\}_{n \in \mathbb{N}_0, \, k \in \mathbb{N}} \longrightarrow h_z(r, \vartheta, \varphi) = -\frac{e^{-\sqrt{z}R}}{4\pi R} \frac{j_0(\sqrt{-z}\,r)}{j_0(\sqrt{-z}\,R)} \tag{69}$$

The following theorem characterize the spectrum of H_α.

12

Theorem 7 *Let H_α be defined by (23)-(24) and (55) and denote with σ_α its spectrum. For any $\alpha \in \mathbb{R} \setminus (0, -4\pi R]$ we have*

$$\sigma_\alpha = \{\lambda_{n,k}\}_{n,k\in\mathbb{N}} \cup \{\zeta_n\}_{\substack{n\in\mathbb{N} \\ n \ odd}} \tag{70}$$

with $\zeta_n \in \mathbb{R}^+$, $\{\lambda_{n,k}\}_{n,k\in\mathbb{N}} \cap \{\zeta_n\}_{\substack{n\in\mathbb{N} \\ n \ odd}} = \varnothing$ and

$$\lim_{\substack{n\to\infty \\ n \ odd}} \left(\sqrt{\zeta_n} - \frac{n\pi}{2R} \right) = 0 \tag{71}$$

For $\alpha \in (0, -4\pi R]$ the spectrum σ_α acquires a negative point

$$\sigma_\alpha = \{\lambda_{n,k}\}_{n,k\in\mathbb{N}} \cup \{\zeta_n\}_{\substack{n\in\mathbb{N} \\ n \ odd}} \cup \{\zeta_{-1}\} \tag{72}$$

with $\zeta_{-1} < 0$. In the case $\alpha = 0$, the set σ_0 is given by

$$\sigma_0 = \{\lambda_{n,k}\}_{n,k\in\mathbb{N}} \cup \{\eta_n\}_{n\in\mathbb{N}} \tag{73}$$

where $\eta_n \in \mathbb{R}^+$, $\{\lambda_{n,k}\}_{n,k\in\mathbb{N}} \cap \{\eta_n\}_{n\in\mathbb{N}}$ are the solutions of

$$\frac{\sqrt{\eta_n} \sin 2\sqrt{\eta_n} R}{1 - \cos 2\sqrt{\eta_n} R} = 0 \quad \forall n \tag{74}$$

Proof. Due to the definition $R_z^\alpha = \frac{1}{H_\alpha + z}$, the spectral points of H_α coincide with the singularities of the operators R_z^α, w.r.t. the variable z, modulo a change of sign. From (64) we see that $R_z^\alpha \varphi$ can be ill defined both for $z \in \{-\lambda_{n,k}\}_{n\in\mathbb{N}_0, k\in\mathbb{N}}$ as for the zeroes of the function

$$f^\alpha(z) = \alpha + \frac{\sqrt{z}}{4\pi} + h_z(\underline{0}) \tag{75}$$

moreover we notice that, as it has been shown in Lemma 5, $h_z(\underline{0})$ is singular in the limit $z \to -\lambda_{n,k}$; then none of these points may coincide with a zero of $f^\alpha(z)$; this circumstance allows us to consider the two cases separately. Concerning the first case, $z \in \{-\lambda_{n,k}\}_{n\in\mathbb{N}_0, k\in\mathbb{N}}$, Theorem 6 (with relation (65)) exclude the points $\{-\lambda_{0,k}\}_{k\in\mathbb{N}}$ from the singularities of $R_z^\alpha \varphi$, from which it follows

$$\{-\lambda_{n,k}\}_{n,k\in\mathbb{N}} \in \sigma_\alpha$$

In order to study the zeroes of (75), we exploit definition (69) - for $z \in \mathbb{C} \setminus \{-\lambda_{n,k}\}$ - and the properties of $j_0(x) = \frac{\sin x}{x}$, to write $f^\alpha(z)$ in the form: $f^\alpha(z) = \alpha + \frac{\sqrt{z}}{4\pi} + \frac{1}{4\pi} \frac{2\sqrt{z}}{e^{2\sqrt{z}R} - 1}$; then the equation $f^\alpha(z) = 0$ reads as

$$\alpha + \frac{\sqrt{z}}{4\pi} + \frac{1}{4\pi} \frac{2\sqrt{z}}{e^{2\sqrt{z}R} - 1} = 0 \tag{76}$$

Setting $z = -\xi$ in equation (76), we recover the equation for the eigenvalues of operator H_α

$$\alpha + \frac{i\sqrt{\xi}}{4\pi} + \frac{1}{4\pi} \frac{2i\sqrt{\xi}}{e^{2i\sqrt{\xi}R} - 1} = 0 \tag{77}$$

The selfadjointness of H_α, allows us to expect only real solutions for (77). We need to distinguish between different situations:

13

1. $\alpha \neq 0$; $\xi \geq 0$. (77) can be written in the form:

$$\frac{\sqrt{\xi}}{4\pi\,\alpha} = \frac{\cos 2\sqrt{\xi}R - 1}{\sin 2\sqrt{\xi}R} \tag{78}$$

The solutions of this equation are the intersection points between the two curves corresponding to the right and left hand side of (78). In Figure 1, we show their behavior, w.r.t. the variable $\sqrt{\xi}$, when the conditions: $\alpha > 0$, $4\pi\,\alpha = \frac{1}{5}$, and $R = 1$ are assumed
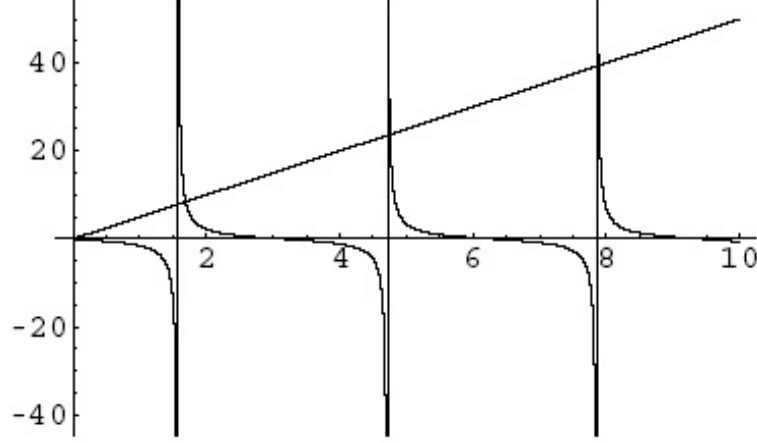

Figure 1

In both cases $\alpha > 0$ and $\alpha < 0$, the intersection points forms an increasing sequence of non negative values $\{\zeta_n\}_{\substack{n \in \mathbb{N} \\ n\ odd}}$ such that:

$$\zeta_1 = 0 \tag{79}$$

and

$$\lim_{\substack{n \to \infty \\ n\ odd}} \left(\sqrt{\zeta_n} - \frac{n\pi}{2R} \right) = 0 \tag{80}$$

2. $\alpha \neq 0$; $\xi < 0$. (77) can be written in the form

$$\alpha + \frac{\sqrt{|\xi|}}{4\pi} + \frac{1}{4\pi}\frac{2\sqrt{|\xi|}}{e^{2\sqrt{|\xi|}R} - 1} = 0 \Rightarrow \frac{\sqrt{|\xi|}}{4\pi\,\alpha} = \frac{1 - e^{2\sqrt{|\xi|}R}}{1 + e^{2\sqrt{|\xi|}R}} \tag{81}$$

The solutions, defined by the intersection points of the two curves, are such that

$$\begin{array}{ll} \alpha \geq -\left(4\pi R\right)^{-1} & \text{no solution} \\ \alpha \in \left(-\infty, -\left(4\pi R\right)^{-1}\right) & \sqrt{|\zeta_{-1}|} \end{array} \tag{82}$$

In Figure 2 we show an example of the second case, $\alpha \in \left(-\infty, -\left(4\pi R\right)^{-1}\right)$
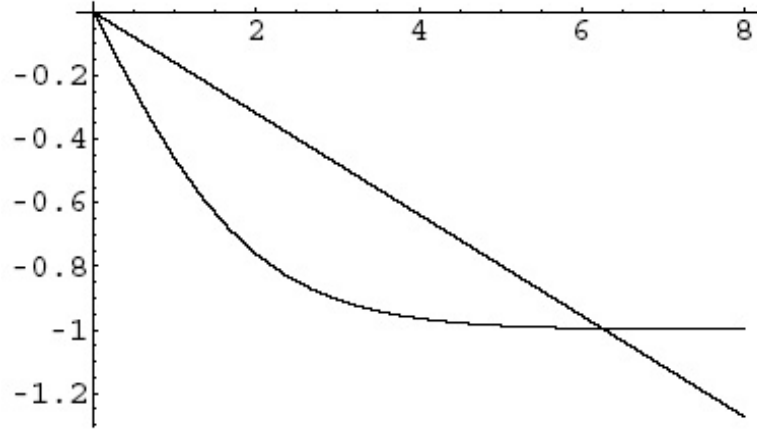
14

Figure 2

3. $\alpha = 0$; $\xi > 0$. Equation (78) becomes

$$\frac{\sqrt{\xi}\sin 2\sqrt{\xi}R}{1 - \cos 2\sqrt{\xi}R} = 0 \tag{83}$$

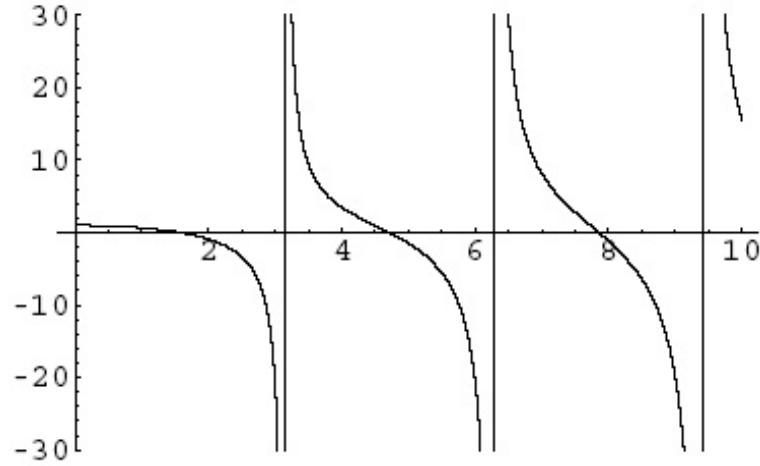which has infinitely many solutions; in Figure 3, the l.h.s. of (83) is plotted w.r.t. the variable $\sqrt{\xi}$

Figure 3

4. $\alpha = 0$; $\xi < 0$. Equation (78) becomes:

$$\sqrt{|\xi|}\left(1 + \frac{2}{e^{2\sqrt{|\xi|}R} - 1}\right) = 0 \tag{84}$$

which has no solution. ∎

The eigenfunctions of H_α, related to the spectral sets (70)-(73), can be obtained directly from definition (59). Consider for instance the action of H_α on the vectors $\psi_{n,m,k}$, $n \neq 0$: by

15

construction, these functions belong to the operator domain and have null charge, from which it follows

$$H_\alpha \psi_{n,m,k} = -\Delta \psi_{n,m,k} = \lambda_{n,k} \psi_{n,m,k} \qquad \forall n \neq 0 \tag{85}$$

Then the set spanned by $\{\psi_{n,m,k}, \ m \in \mathbb{Z} \cap [-n,n]\}$ represents the autospace of H_α related to the eigenvalue $\lambda_{n,k}$.

On the other hand, if we consider a spectral point $\lambda \in \sigma_\alpha \setminus \{\lambda_{n,k}\}_{n,k \in \mathbb{N}}$, from (59) it follows that the corresponding solution of the eigenvalue problem is $q \mathcal{G}_0^{-\lambda}$ with $q \in \mathbb{C}$.

5   Coupling one particle with a quantum bit

In this section we briefly sketch how point interaction models can be used in order to describe an information flow between two interacting quantum systems. To this aim, making use of the results obtained above, we shall give a complete characterization of the family of point interactions coupling a quantum particle - confined in a finite volume of $\mathbb{R}^3$ - with a two level quantum system (q-bit).

Let Ω be the ball of radius R centered in the origin of $\mathbb{R}^3$ and consider the symmetric operator

$$\begin{cases} T_0 = H_0 \otimes \mathbb{I}_{\mathbb{C}^2} + \mathbb{I}_{L^2(\Omega)} \otimes U \\ D(T_0) = D(H_0) \otimes \mathbb{C}^2 \end{cases} ; \quad U = \begin{pmatrix} E_+ & 0 \\ 0 & E_- \end{pmatrix}, \ E_\pm \in \mathbb{R} \tag{86}$$

where H_0 is defined by (5) while U is the Hamiltonian associated to the q-bit. The selfadjoint extensions of T_0 shall describe zero range interactions, acting in the origin of the ball Ω, between the particle and the quantum bit. The construction of these extensions will be performed along the same line followed in the previous Sections. From Lemma 2 follows that the defect spaces of T_0 are

$$\mathcal{H}_+ = l.s. \left\{ \sum_{\sigma=\pm} \mathcal{G}_0^{-i-E_\sigma} \otimes \chi_\sigma \right\}; \quad \mathcal{H}_- = l.s. \left\{ \sum_{\sigma=\pm} \mathcal{G}_0^{i+E_\sigma} \otimes \chi_\sigma \right\}$$

where $\chi_+ = (1,0)$, $\chi_- = (0,1)$ are the eigenvectors of the matrix A, while the functions $\mathcal{G}_0^z$ are defined by (61)-(69). Moreover, let $\Psi = \sum_{\sigma=\pm} \psi_\sigma \otimes \chi_\sigma$, $\psi_\sigma \in L^2(\Omega)$, be a generic vector in $D(T_0^*)$; we define the maps $\Lambda_{1,2} : D(T_0^*) \to \mathbb{C}^2$ as follows

$$(\Lambda_j \Psi)_\sigma = \Gamma_j \psi_\sigma, \quad j = 1,2 \tag{87}$$

$$\Gamma_1 \psi_\sigma = \lim_{\underline{x} \to \underline{0}} 4\pi \, |\underline{x}| \, \psi(\underline{x}) \tag{88}$$

$$\Gamma_2 \psi_\sigma = \lim_{\underline{x} \to \underline{0}} \left(\psi(\underline{x}) - \frac{\Gamma_1 \psi_\sigma}{4\pi \, |\underline{x}|} \right) \tag{89}$$

Proceeding as in Theorem 3, it is easy to show that $\left(\mathbb{C}^2, \Gamma_1, \Gamma_2\right)$ form a boundary value space for the operator T_0. Proposition 1 implies that all selfadjoint extensions of T_0 are parametrized by couples of matrices $A, B \in \mathbb{C}^{2,2}$ fulfilling the conditions $[I]$ and $[II]$ (see Section 2); each extension T^{AB} is a restriction of the adjoint T_0^* to those vectors $\psi \in D(T_0^*)$ satisfying the relation

$$A\Lambda_1 \psi = B\Lambda_2 \psi \tag{90}$$

The following Theorem provides an explicit representation of T^{AB}

Theorem 8 *Let $A, B \in \mathbb{C}^{2,2}$ satisfying the conditions [I] and [II]; for any $\lambda \in \mathbb{C}\backslash\mathbb{R}$, the selfadjoint extension T^{AB}, corresponding to the couple A, B, is described as follows*

$$D(T^{AB}) = \{\Psi = \sum_{\sigma=\pm} \left(\phi_\sigma^\lambda + q_\sigma \mathcal{G}_0^\lambda\right) \otimes \chi_\sigma | \ \phi_\sigma^\lambda \in H^2 \cap H_0^1(\Omega);$$

$$q_\sigma = (\Lambda_1 \Psi)_\sigma \, ; \ \phi_\sigma^\lambda(\underline{0}) = \sum_{\sigma'=\pm} \left[\left(h_\lambda(\underline{0}) + \frac{\sqrt{\lambda}}{4\pi}\right)\mathbb{I} + B^{-1}A\right]_{\sigma\sigma'} q_{\sigma'}\}$$

$$T^{AB}\Psi = \sum_{\sigma=\pm} \left(-\Delta\phi_\sigma^\lambda - \lambda q_\sigma \mathcal{G}_0^\lambda\right) \otimes \chi_\sigma + \sum_{\sigma=\pm} \left(\phi_\sigma^\lambda + q_\sigma \mathcal{G}_0^\lambda\right) \otimes U\chi_\sigma$$

Moreover given any $\Phi = \sum_{\sigma=\pm} \varphi_\sigma \otimes \chi_\sigma$ in $L^2(\Omega) \otimes \mathbb{C}^2$, the action of the resolvent operator $R_z^{AB} = \frac{1}{T^{AB}+z}$ on Φ is

$$R_z^{AB}\Phi = \sum_{\sigma=\pm} \left(R_z\varphi_\sigma + \sum_{\sigma',\nu=\pm} \left(B\left(h_\lambda(\underline{0}) + \frac{\sqrt{\lambda}}{4\pi}\right)\mathbb{I} + A\right)_{\sigma\sigma'}^{-1} B_{\sigma'\nu} R_z\varphi_\nu(\underline{0}) \mathcal{G}_0^\lambda\right) \otimes \chi_\sigma$$

Proof. The proof is easily obtained following the same line of Theorem 4. ∎

In the perspective of applications, we consider of particular interest the subfamily of selfadjoint extensions T^{AB} described by the conditions

$$A = \begin{pmatrix} \alpha_+ & 0 \\ 0 & \alpha_- \end{pmatrix}; \quad B = \mathbb{I} \tag{91}$$

These operators, which will be denoted in the following as $T_{\{\alpha_+,\alpha_-\}}$, are defined by

$$D(T_{\{\alpha_+,\alpha_-\}}) = \left\{\Psi = \sum_{\sigma=\pm} \psi_\sigma \otimes \chi_\sigma \, \middle| \, \psi_\sigma \in D(H_{\alpha_\sigma})\right\} \tag{92}$$

$$T_{\{\alpha_+,\alpha_-\}}\Psi = \sum_{\sigma=\pm} H_{\alpha_\sigma}\psi_\sigma \otimes \chi_\sigma + \sum_{\sigma=\pm} \psi_\sigma \otimes U\chi_\sigma \tag{93}$$

where H_{α_σ} is an Hamiltonian with a point interaction acting in the origin of the ball Ω with strength α_σ (see the definitions (58)-(59) and Theorem 8).

Let us consider a quantum mechanical system consisting of a confined particle interacting with a quantum bit through the Hamiltonian operator $T_{\{\alpha_+,\alpha_-\}}$. The specific feature of this model rests upon the fact that the particle may follow a different dynamics - generated respectively by the Hamiltonians H_{α_+} and H_{α_-} - depending on the state of the q-bit. At the same time, the latter evolves freely, independently of the motion of the particle. Therefore, in the time evolution of this system, we shall observe a flow of information from the q-bit to the particle without energy exchanges. The extension of this model to the case of N confined quantum particles, the analysis of the implications between the lack of coherence of the q-bit and the information flow to its environment, as well as the construction of point interaction models of quantum measurement apparata, will be considered in further work.

References

[1] F.A. Berezin and L.D. Fadeev. Remark on the Schrödinger equation with singular potential. *Dokl. Akad. Nauk. SSSR,* 137, 1011-1014, 1961

[2] S. Albeverio, F. Gesztesy, R Högh-Krohn and H. Holden. Solvable Models in Quantum Mechanics. *Springer-Verlag, New York,* 1988.

[3] W. Caspers and G. Sweers. Point interactions on bounded domains. *Proc. R. Soc. Edinburgh*, 124A, 917-926, 1994.

[4] C. Cacciapuoti, R. Carlone, R. Figari. Spin-dependent point potentials in one and three dimensions. *J. Phys. A: Math. Gen.,* 40, 249-261, 2007.

[5] K. Pankrashkin. Resolvents of self-adjoint extensions with mixed boundary conditions. *Rep. Math. Phys.,* 58, 207-221, 2006.

[6] V. I. Gorbachuk and M. L. Gorbachuk, *Boundary Value Problems for Operator Differential Equations.* Dordrecht: Kluwer, 1991.

[7] Reed M and Simon B. *Methods of Modern Mathematical Physics vol II: Fourier Analysis, Self-Adjointness.* Academic Press, 2002.

[8] S. Albeverio, K. Pankrashkin. A remark on Krein's resolvent formula and boundary conditions. *J. Phys. A: Math. Gen.,* 38, 4859-4864, 2005.

[9] B. S. Pavlov. The Theory of Extensions and Explicitly-Solvable Models. *Usp. Mat. Nauk.* 42, 99–131, 1987. English transl.: *Russ. Math. Surv.* 42, 127–168 (1987).

[10] P. Kurasov and A. Posilicano. Finite speed of propagation and local boundary conditions for wave equations with point interactions. Preprint Nr. 10, Department of Mathematics, Lund Institute of Technology, 2004.